# Aura-TES L2 Products: Version 7 Data Quality Description

## Overview of Current Data Quality Status

This is a preliminary report on data quality of TES Version 7 data (V007, files ending in F08_11). New standard TES products in V007 are two new species, peroxyacetyl nitrate (PAN) and carbonyl sulfide (OCS). V007 continues the same standard TES products as V006, including TES L1B radiances, ozone, carbon monoxide, atmospheric temperature, water vapor, HDO, methane, sea surface temperature, cloud properties, carbon dioxide, formic acid (HCOOH), methanol ($CH_3OH$), ammonia, and the ozone band Instantaneous Radiative Kernel (IRK). For water vapor and atmospheric temperature initial guess and constraint, the Global Modeling and Data Assimilation Office (GMAO) GEOS-5.12.4 model is used. Level 2 data nadir products are all validated and usable in scientific analyses. Details on the validation of TES standard products are available in the TES V007 Data Validation Report (Herman et al., 2018).

The subsections below give a brief overview of the latest data quality analysis of TES V007 and/or V006 data. In order to successfully interpret TES data, one must account for the variable vertical sensitivity of the TES product and the *a priori* constraints used to help convert measured radiances to vertical profiles of tropospheric composition. Biases in the data can also vary with altitude. Comparisons between TES data and earth atmosphere models can also be challenging because of possible logarithmic differences between the data product, *a priori*, and model fields.

We therefore recommend that the scientist interested in TES data read Chapter 9 of the TES Data User's Guide (Herman and Kulawik, 2013) on how to interpret and use TES data and any published papers in which the data are used (all published papers using TES data are listed on the TES website). For example, these papers will discuss how biases are addressed or how logarithmic differences between TES data and model fields affect scientific interpretation. All of the TES validation papers and other publications are available at the TES publications web site.

Users should also read the data quality statement listed below. For most scientific applications a data user should select data using the master data quality flag ("speciesretrievalquality") and a check on the sensitivity with the DegreesOfFreedomForSignal data field. If these checks are removing too much data over the area of interest then the user should contact a member of the TES science team on how to use a subset of flags.

## Data Quality and Validation Status for TES Level 1B Radiance Data Product

Though this report is focused primarily on the TES Level 2 data products, it is important to understand that the L1B radiance products have also undergone a rigorous validation as reported in Shephard et al. (2008) and in the TES Validation Report V003 (Osterman et al., 2007). The fundamental measurement of the Tropospheric Emission Spectrometer (TES) on board the Aura spacecraft is upwelling infrared spectral radiances. Accurate radiances are critical for trace gas profile retrievals for air quality as well as sensitivity to climate processes. For example, any radiometric systematic errors (*e.g.* calibration) not addressed in the L1B radiances will propagate as errors into the retrieved atmospheric parameters (Bowman et al., 2006; Worden et al., 2004). Connor et al (2011) showed that the TES relative radiometric calibration was extremely stable over the time period used in their analysis: 2005 to 2009.

In April 2010, TES implemented a new strategy for observing and processing calibration measurements (see Section 4 of the Version 5 Data Validation Report, Herman et al., 2012). In order to validate TES spectra processed with the new calibration strategy, and to check comparisons of TES with AIRS over the entire TES data record from 2004 to present, we developed a more automated comparison tool based on the methods used for TES/AIRS comparisons in Shephard et al. (2008). Given the differences in ground footprints for TES and AIRS, comparisons are only meaningful for clear-sky, ocean scenes. Results for April 2009 (old calibration approach) compared to April 2010 (new calibration approach) are not significantly different, which suggests the new approach provides the same radiance accuracy as before.

# Data Quality and Validation Status for TES Level 2 Data Products

## New Products PAN and OCS

## Nadir Peroxyacetyl Nitrate (PAN)

Peroxyacetyl nitrate (PAN) is a new product in TES V007. PAN may show large variation on relatively small spatial scales. Ideally, the PAN product would be validated using comparisons with coincident in situ measurements. At this time, sufficient coincidences for robust validation are not available. However, prototype TES PAN retrievals have been previously examined for the existence of expected features in the PAN fields, and these prototype retrievals have already been utilized in peer-reviewed publications. Therefore, we have performed a preliminary assessment of the V007 PAN product by comparing to datasets that have been utilized in two existing publications.

Payne et al. [2014] showed examples of elevated CO and PAN in boreal burning plumes (previously identified by Alvarado et al. [2010]) seen in TES special observations made during the July 2008 phase of the ARCTAS campaign. These plume examples showed strong evidence for PAN enhancements in fire plumes and demonstrated that it was possible for adjacent TES pixels to show sharply different PAN volume mixing ratios. Although coincident aircraft data were not available, the retrieved PAN values, between zero and 1.5 ppbv, were deemed to be reasonable, given the range of PAN values measured from aircraft during the campaign [Alvarado et al., 2010; Roberts et al., 2009]. Payne et al. [2017] showed prototype PAN retrieval results for the Tropics in austral spring, showing a maximum in PAN over the tropical Atlantic, a feature that had been predicted by models and also previously observed using limb-sounding satellite measurements.

## Nadir Carbonyl Sulfide (OCS)

Carbonyl sulfide is a new standard product in TES V007. The data quality of TES OCS product has been assessed through comparisons between TES OCS and aircraft measurements collected during five HIAPER Pole-to-Pole (HIPPO) campaigns during months of January, March to April, June to July, August to September, and November.

The latitudinal distribution in TES OCS is consistently varying with HIPPO observations with root-mean-square of the differences for individual comparison range from 3 to 7 ppt. The global bias is approximately 1.46 ppt with an error standard deviation of about 5.97 ppt. The correlation coefficients between TES OCS and HIPPO for five campaigns are on average of 0.8.

## Nadir Ozone

The retrieval algorithm for TES V007 is largely the same as that utilized for the V006 data set. There were few changes in the retrieval code for this latest version of the TES that affect the ozone retrievals and the comparisons to ozonesondes support that conclusion. The changes to the retrieval system are mostly in the Level 1B steps, including updates to radiance spike detection and path difference thresholds. Previous versions of the TES Validation Report have shown the consistency in the ozone retrievals as the retrieval system has evolved.

TES V007 nadir ozone profiles have been compared with ozonesonde measurements archived in the World Ozone and Ultraviolet Radiation Data Center (WMO/GAW, 2017). As of the writing of this document, the TES ozone retrievals have been matched with ozonesonde data with coincidence criteria of ±9 hours and 300 km distance and a limit on the cloud optical depth of a value less than 2.0. The comparison of the differences between the V007 ozone retrievals with the ozonesondes and corresponding V006 data show very consistent values. Looking at the mean values for 2006, the V007 data agreed slightly better with the ozonesondes in the troposphere by about 4-6 percent. Checks for 2007 also showed better agreement for the V007 data with ozonesondes. In both cases, there were fewer comparisons for V007 than V006 due to the incomplete processing of the V007 data set. The percent differences generally show an improvement when compared to Nassar et al. (2008) and Boxe et al. (2010).

## Nadir Carbon Monoxide

Comparisons have been carried out between TES carbon monoxide retrievals and those from a variety of satellite and aircraft instruments. Global patterns of carbon monoxide as measured by TES are in good qualitative agreement with those seen by MOPITT on the NASA Terra satellite. Comparisons of profiles of CO between TES and MOPITT show better agreement when a priori information is accounted for correctly. TES carbon monoxide agrees to within the estimated uncertainty of the aircraft instruments, including both errors and the variability of CO itself. TES V007 CO VMRs are slightly higher than V006 in the upper troposphere. This is also reflected in

TES-MOPITT comparisons so that the lower bias of TES in V006 comparison is no longer the case.

## Nadir Carbon Dioxide

TES $CO_2$ is retrieved between 40S and 45N, with average cloud optical depth < 0.5, among other tests, for good quality. On average, TES $CO_2$ has an average of 0.65 degree of freedom for signal (DOFS) – with the most DOFS for daytime land cases (which can be on the order of 1 DOFS) and the least for nighttime or winter land cases (which can be on the order of 0.3 DOFS). Ocean targets (day or night) have intermediate DOFS with about 0.8 DOFS. The averaging kernel indicates sensitivity between the surface to above 100 hPa, with the most sensitivity between about 700 and 300 hPa, peaking at about 650 hPa. Although a profile is retrieved, there is very little independent information at the different profile levels and it is necessary to utilize the provided averaging kernel when using TES data. Most of the validation has been performed at the 510 hPa pressure level. TES V007 $CO_2$ is compared with aircraft vertical profiles over the Pacific from the HIAPER Pole-to-Pole Observation (HIPPO) program (Wofsy, 2011). Comparisons over land at the SGP ARM site require the full TES record to be processed and will be done when the V007 record is complete.

Comparisons to HIPPO data show that V007 TES data have improved bias over V006 (for all campaigns except HIPPO 3S), but have somewhat worse standard deviation differences versus HIPPO. Individual TES soundings have error of about 6 ppm, about 2.3 ppm for 10-observation averages, 1.7 ppm for 20-observation averages. The error has a random component that reduces with averaging and a correlated component that does not reduce with averaging. Errors tend to be correlated for close locations and times, and it is recommended to use TES data averaged in 10 degree by 10 degree by 1 month averages, both to mitigate correlated errors and reduce errors to useful levels.

## Nadir Atmospheric Temperature

TES V007 nadir temperature (TATM) retrievals have been compared with nearly coincident radiosonde measurements from the NOAA ESRL global radiosonde database. Generally, V007 TATM is very similar to the previous V006 data. For TES V007 TATM minus $T_{radiosonde}$ (with averaging kernel applied), the bias is less than ±0.25 K in the lower troposphere, decreasing to -0.7 K in the upper troposphere. The rms is less than 1 K in the stratosphere and upper troposphere, increasing to 1.7 K in the lower troposphere. In clear sky conditions (average cloud effective optical depth less than 0.1), the bias improves in the lower troposphere but increases to +0.5 K at the 464 hPa pressure level.

To evaluate the retrieval stability the monthly mean and standard deviation of the TATM residual between TES V005 and the Global Modeling and Data Assimilation Office (GMAO) GEOS-5.2 model, which provides the first guess and a priori for the TATM retrieval, were calculated. The statistics for both Tropical Pacific and Northern Atlantic Ocean regions indicate only minor month-to-month variability and no substantial trends over a five-and-a-half year period of 2006 through 2011. The standard deviation of the residual was generally smaller than the standard deviation of the GMAO GEOS-5.2 but larger than the TES estimated measurement error. Overall, based on this analysis it appears that the TES retrieval quality has remained stable over the years inspected, 2006 through 2011.

## Nadir Water Vapor

TES V007 $H_2O$ has been compared to V006 $H_2O$. Individual retrievals show differences between V007 and V006: these changes are largely due to the new a priori constraint, GMAO GEOS 5.12.4 (for TES V007) versus 5.9.1 (TES V006). On average, though, the mean differences are insignificant. The user should select data using the master data quality flag ("speciesretrievalquality") and filter by DOFS.

## Nadir HDO/$H_2O$

TES V007 estimates of HDO/$H_2O$ have been compared to V006. There is essentially a zero-mean difference between the versions and the uncertainty calculation between versions are consistent. V007 HDO/$H_2O$ shows considerable sensitivity to the isotopic composition of water vapor with typically DOFS~2 in the tropics and DOFS~1 at high latitudes. This increased sensitivity allows the TES estimates to resolve lower tropospheric and mid-tropospheric variability of the HDO/$H_2O$ vapor ratio (see Worden et al., 2012) with the expense of increased uncertainty over tropical oceans.

## Nadir Ammonia ($NH_3$)

Ammonia ($NH_3$) is a standard product in TES V007. The V007 algorithm update had little impact on the retrieved profiles, with insignificant bias between versions V007 and V006. TES $NH_3$ provides useful information over regions with moderate to strong $NH_3$ sources. Due to the sparse TES coverage and the weak signal from $NH_3$, single TES observations have large uncertainties, except over regions with very high $NH_3$ concentrations. However, spatial and temporal averages show good correlation with chemical transport model (CTM) output and with *in situ* measurements.

## Formic Acid (HCOOH)

TES V007 formic acid (HCOOH) provides useful information over regions with strong HCOOH sources, e.g. biomass burning events. Due to the sparse TES coverage and the weak signal from HCOOH, single TES observations have large uncertainties. However, spatial and temporal averages show good correlation with CTM output and with the very limited set of co-located *in situ* measurements.

## Methanol ($CH_3OH$)

TES methanol ($CH_3OH$) has a weak signal and an *a priori* distribution chosen as a function of location and date. The information content of the retrieval is quite low, but seasonal averages over large regions do provide useful information for evaluating CTMs.

## Nadir Methane

Previously, TES V006 $CH_4$ was validated against aircraft observations from all five missions of the HIAPER Pole-to-Pole Observations (HIPPO) campaign. Comparisons were performed for both the $CH_4$ profiles reported in the Level 2 files, and for $N_2O$-corrected $CH_4$ profiles. (See Worden et al. [2012] for details of the $N_2O$ correction.) These comparisons are described in Alvarado et al. [2015], who found a high overall bias in the TES V006 $CH_4$ retrievals. The bias for TES V006 $CH_4$ relative to HIPPO measurements between 50S and 50N was 56.9 ppbv (25.7 ppbv after the $N_2O$ correction) for upper tropospheric representative values and 27.3 ppbv (28.4 ppbv after the $N_2O$ correction) for lower tropospheric representative values.

The TES V007 $CH_4$ retrieval approach is the same as V006. There were no changes in the spectroscopy for either $CH_4$ or $N_2O$ (or for $H_2O$ or HDO, significant spectral interferents that are jointly retrieved with $CH_4$ and $N_2O$ in the V006 and V007 algorithm). There were no changes in the *a priori* and initial guess for $CH_4$ or $N_2O$. There were updates to the GMAO water vapor and temperature profiles used as initial guess and a priori for those quantities (to GMAO GEOS-5.12.4). Using 37 TES global surveys from the time periods of the HIPPO campaign, we find that the mean difference between V006 and V007 is less than 3 ppbv at all altitudes for both uncorrected and $N_2O$-corrected profiles, with standard deviation less than 30 ppbv at all altitudes. We speculate that the variability in the differences between V006 and V007 $CH_4$ arises from the updates to the GMAO water vapor and temperature profiles.

## Ozone Band Instantaneous Radiative Kernel (IRK)

TES Instantaneous Radiative Kernel (IRK) just for ozone over 9.6-micron ozone band was a standard product in TES V006 using a 3-point Gaussian integration method. In TES , we use a 5-point Gaussian integration, a computationally more expensive but more accurate method, to compute IRK and expand the IRK products to include 1) 9.6-micron band TOA flux (980 – 1020.2 /cm), 2) both IRK and LIRK (logarithm IRK) for $O_3$ and water vapor ($H_2O$), 3) LIRK for cloud optical depth (COD), cloud top pressure (CTP), and emissivity (EMIS), and 4) IRK for atmospheric temperature (TATM) and surface temperature (TSUR) (see Table 1). These products have been validated individually with prototype (IDL) code calculations (Kuai et al., 2017) using one global survey observations.

The statistics (the mean and one standard deviation) for the fractional differences between PGE and prototype of all IRK products calculated using the same Jacobians for integration are showed to have negligible differences (1E-06% ± 3E-06%). The global pattern for all products are well replicated by PGE algorithm.

## Nadir Surface Temperature (Sea Surface Temperature)

TES retrieves surface (skin) temperature as standard product. Over ocean this amounts to a sea surface temperature (SST). TES retrievals of SST rely on validation of V003. Comparisons of TES V003 data to the Reynolds Optimally Interpolated (ROI) sea surface temperature product between January 2005 and July 2008 show very small biases. The TES V003 observations have a bias relative to ROI data for night/day of -0.20/0.04 K.

## TES Nadir Cloud Products

Here we report on version V005 TES cloud products, which have been validated by comparing TES estimates of effective cloud optical depth and cloud top height to those from the Moderate Resolution Imaging Spectroradiometer (on EOS) (MODIS), the Atmospheric Infrared Sounder (AIRS), and to simulated data. The radiance contribution of clouds is parameterized in TES retrievals in terms of a set of frequency-dependent nonscattering effective optical depths and a cloud height. This unique approach jointly retrieves cloud parameters with surface temperature, emissivity, atmospheric temperature, and trace gases such as ozone from TES spectral radiances. We calculate the relationship between the true optical depth and the TES effective optical depth for a range of single-scatter albedo and phase functions to show how this varies with cloud type. We estimate the errors on retrieved cloud parameters using a simulated data set covering a wide range of cloud cases. For simulations with no noise on the radiances, cloud height errors are less than 30 hPa, and effective optical depth follows expected behavior for input optical depths of less than 3. When random noise is included on the radiances, and atmospheric variables are included in the retrieval, cloud height errors are approximately 200 hPa, and the estimated effective optical depth has sensitivity between optical depths of 0.3 and 10. The estimated errors from simulation are consistent with differences between TES and cloud top heights and optical depth from MODIS and AIRS.

## Limb products

Limb products have not changed from V004, see the V004 quality statement for descriptions for these.

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